3-Hydroxyphenylacetic acid
621-37-4 | DTXSID90211148

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 261 °C

Global applicability domain: Inside

Local applicability domain index: 2.57e-01

Confidence level: 4.84e-01

Nearest Neighbors from the Training Set

Image not found
2-Hydroxyphenylacetic acid
Measured: 240
Predicted: 261

Image not found
2-Chlorobenzoic acid
Measured: 287
Predicted: 273

Image not found
Benzoic acid, 4-methoxy-
Measured: 277
Predicted: 279

Image not found
2,5-Dichlorobenzoic acid
Measured: 301
Predicted: 288